

1 Physics 40E handout on Fourier matters

1.1 Fourier Series

I will first consider periodic functions f that obey

$$f(x - L/2) = f(x + L/2) \quad (1)$$

where L is the period. Important examples of these functions are

$$e^{2\pi i n x / L}, \quad n = 0, \pm 1, \pm 2, \dots \quad (2)$$

The idea is first to find the best approximation to a periodic function f using the above exponentials, that is, consider

$$g(x) = \sum_{n=-\infty}^{\infty} g_n e^{2\pi i n x / L} \quad (3)$$

(which is periodic with period L) and find the coefficients g_n for which

$$\Delta = \int_{-L/2}^{L/2} dx |f - g|^2 \quad (4)$$

is as small as possible.

Since g_n is in general complex I will write

$$g_n = u_n + i v_n \quad (5)$$

Then, using

$$\begin{aligned} \left(\frac{\partial |f - g|^2}{\partial u_n} \right) &= - \left(\frac{\partial g^*}{\partial u_n} \right) (f - g) - (f^* - g^*) \left(\frac{\partial g}{\partial u_n} \right) \\ &= -e^{-2\pi i n x / L} (f - g) - (f^* - g^*) e^{-2\pi i n x / L} \\ \left(\frac{\partial |f - g|^2}{\partial v_n} \right) &= - \left(\frac{\partial g^*}{\partial v_n} \right) (f - g) - (f^* - g^*) \left(\frac{\partial g}{\partial v_n} \right) \\ &= i e^{2\pi i n x / L} (f - g) - i (f^* - g^*) e^{2\pi i n x / L} \end{aligned} \quad (6)$$

The minimum of Δ occurs whenever

$$0 = \left(\frac{\partial \Delta}{\partial u_n} \right) = - \int_{-L/2}^{L/2} dx \left[(f - g) e^{-2\pi i n x / L} + (f - g)^* e^{2\pi i n x / L} \right]$$

$$0 = \left(\frac{\partial \Delta}{\partial v_n} \right) = i \int_{-L/2}^{L/2} dx \left[(f - g) e^{-2\pi i n x / L} - (f - g)^* e^{2\pi i n x / L} \right] \quad (7)$$

which imply

$$\int_{-L/2}^{L/2} dx (f - g) e^{-2\pi i n x / L} = 0 \quad \int_{-L/2}^{L/2} dx (f - g)^* e^{2\pi i n x / L} = 0 \quad (8)$$

Note that these are complex conjugate of each other, so I can impose one and the other will be immediately satisfied. Using the first of them I get

$$\begin{aligned} \int_{-L/2}^{L/2} dx f e^{-2\pi i n x / L} &= \int_{-L/2}^{L/2} dx g e^{-2\pi i n x / L} \\ &= \int_{-L/2}^{L/2} dx \sum_{n'=-\infty}^{\infty} g_{n'} e^{2\pi i n' x / L} e^{-2\pi i n x / L} \\ &= \sum_{n'=-\infty}^{\infty} g_{n'} \int_{-L/2}^{L/2} dx e^{2\pi i n' x / L} e^{-2\pi i n x / L} \end{aligned} \quad (9)$$

Now, for $n' \neq n$ I have

$$\begin{aligned} \int_{-L/2}^{L/2} dx e^{2\pi i n' x / L} e^{-2\pi i n x / L} &= \frac{L}{2\pi i (n' - n)} e^{2\pi i (n' - n) x / L} \Big|_{-L/2}^{L/2} \\ &= \frac{L}{2\pi i (n' - n)} [e^{\pi i (n' - n)} - e^{-\pi i (n' - n)}] \\ &= \frac{L}{\pi (n' - n)} \sin[\pi (n' - n)] \\ &= 0 \end{aligned} \quad (10)$$

therefore

$$\begin{aligned} \int_{-L/2}^{L/2} dx f e^{-2\pi i n x / L} &= \sum_{n'=-\infty}^{\infty} g_{n'} \int_{-L/2}^{L/2} dx e^{2\pi i n' x / L} e^{-2\pi i n x / L} \\ &= g_n \int_{-L/2}^{L/2} dx e^{2\pi i n x / L} e^{-2\pi i n x / L} \\ &= L g_n \end{aligned} \quad (11)$$

since only the term $n' = n$ is not zero.

The best approximation to f is then

$$\sum_{n=-\infty}^{\infty} g_n e^{2\pi i n x / L}, \quad g_n = \frac{1}{L} \int_{-L/2}^{L/2} dx f e^{-2\pi i n x / L} \quad (12)$$

In fact it can be shown that for functions such that f , df/dx and d^2f/dx^2 have at most finite jumps this best approximation is equal to f ,

$$f(x) = \sum_{n=-\infty}^{\infty} g_n e^{2\pi i n x / L}, \quad g_n = \frac{1}{L} \int_{-L/2}^{L/2} dx f(x) e^{-2\pi i n x / L} \quad (13)$$

1.1.1 Example

Consider the case $L = 2\pi$ and the function

$$\begin{aligned} f(x) &= +1 \text{ for } 0 < x < \pi \\ &= -1 \text{ for } -\pi < x < 0 \\ &= \frac{x}{|x|} \end{aligned} \quad (14)$$

From the definition

$$\begin{aligned} g_n &= \frac{1}{2\pi} \left(\int_0^\pi e^{-iny} dy - \int_{-\pi}^0 e^{-iny} dy \right) \\ &= \frac{1}{2\pi} \left(\frac{e^{-in\pi} - 1}{-in} - \frac{1 - e^{+in\pi}}{-in} \right) \\ &= \frac{(-1)^n - 1}{-in\pi} \\ g_{2k+1} &= -\frac{2i}{(2k+1)\pi} \\ g_{2k} &= 0 \end{aligned} \quad (15)$$

Substituting I find

$$f(x) = \frac{4}{\pi} \left(\sin x + \frac{1}{3} \sin(3x) + \frac{1}{5} \sin(5x) + \dots \right) \quad (16)$$

The way the sum converges can be seen in figure 1

Now in the interval $0 < x < \pi$ I then get

$$\frac{\pi}{4} = \left(\sin x + \frac{1}{3} \sin(3x) + \frac{1}{5} \sin(5x) + \dots \right) \quad (17)$$

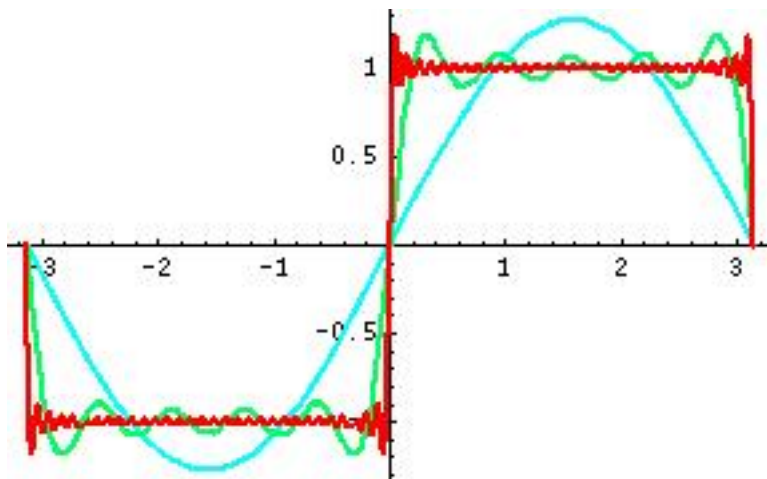


Figure 1: Fourier series approximation to $x/|x|$ for $|x| < \pi$. The blue curve corresponds to taking only the first term, green curve taking the first 4 terms, the red curve taking the first 30 terms.

so that, putting $x = \pi/2$,

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \cdots \quad (18)$$

Next, integrating 17 from 0 to x gives

$$\frac{\pi}{4}x = (1 - \cos x) + \frac{1}{3^2} [1 - \cos(3x)] + \frac{1}{5^2} [1 - \cos(5x)] + \cdots \quad (19)$$

and again putting $x = \pi/2$,

$$\frac{\pi^2}{8} = 1 + \frac{1}{9} + \frac{1}{25} + \cdots \quad (20)$$

1.1.2 Exercises

1. Expand $f(x) = \sin(|x|)$, $|x| < \pi$ in a Fourier series
2. Expand the function $f(x) = x$, $|x| < \pi$ in a Fourier series
3. Expand the function $f(x) = \sin(\mu x)$, $|x| < \pi$ in a Fourier series

4. Using equations 17, 19 show that

$$\frac{\pi^3}{32} = 1 - \frac{1}{27} + \frac{1}{125} + \dots \quad (21)$$

5. Use equation 17 to show that

$$\frac{\pi^2}{6} = 1 + \frac{1}{4} + \frac{1}{9} + \frac{1}{16} + \frac{1}{25} + \dots \quad (22)$$

1.2 Fourier Integrals

I will now consider the $L \rightarrow \infty$ limit. To take it I define

$$h = \frac{2\pi}{L} \quad k_n = nh = \frac{2\pi n}{L} \quad (23)$$

then the above expression become

$$\begin{aligned} \frac{2\pi}{h} g_n &= \int_{-L/2}^{L/2} dx e^{-ixk_n} f(x) \\ f(x) &= \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} h \left(\frac{2\pi}{h} g_n \right) e^{ixk_n} \end{aligned} \quad (24)$$

this suggests the definition

$$g(k) = \int_{-\infty}^{\infty} dx e^{-ixk} f(x) \quad (25)$$

so that, as $L \rightarrow \infty$, $(2\pi/h)g_n \rightarrow g(k_n)$. Also the “distance” between to consecutive values of k_n is

$$\delta k = k_{n+1} - k_n = h \quad (26)$$

so that I can write

$$f(x) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \delta k g(k_n) e^{ixk_n} \quad (27)$$

which in the $L \rightarrow \infty$ limit becomes an integral. Collecting results I get

$$\begin{aligned} \mathbf{f}(\mathbf{x}) &= \int_{-\infty}^{\infty} \frac{d\mathbf{k}}{2\pi} \mathbf{g}(\mathbf{k}) e^{i\mathbf{k}\mathbf{x}} \\ \mathbf{g}(\mathbf{k}) &= \int_{-\infty}^{\infty} d\mathbf{x} \mathbf{f}(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}} \end{aligned} \quad (28)$$

In this case one says that f and g are Fourier transforms of each other.

1.2.1 Exercises

1. Find the Fourier transform of the step function

$$f(x) = \begin{cases} 1 & |x| < b \\ 0 & |x| \geq b \end{cases} \quad (29)$$

Plot the result, note that a discontinuity in f generates oscillations in g

2. Find the Fourier transform of the n -th derivative $d^n f/dx^n$ in terms of g , assuming that f and all its derivatives vanish as $|x| \rightarrow \infty$.

Hint: integrate by parts.

3. Find the Fourier transform of $F(x) = f(bx)e^{itx}$ in terms of g , the Fourier transform of f .

Hint: make an appropriate change of variables.

4. Find the Fourier transform of

$$f(x) = Ae^{-bx^2/2} \quad (30)$$

Plot your result; note that there is a relation between the half-widths of f and g and that no strong oscillations are induced in g even though f is localized.

5. Show that if f is even its Fourier transform is

$$g(k) = \int_{-\infty}^{\infty} dx \cos(\mathbf{k}x) f(x) \quad (31)$$

6. Show that if f is odd and real then g is purely imaginary.

1.3 Integral identities

If we have two periodic functions f and F with

$$\begin{aligned} f(x) &= \sum_{n=-\infty}^{\infty} g_n e^{2\pi i n x/L} \\ F(x) &= \sum_{n=-\infty}^{\infty} G_n e^{2\pi i n x/L} \end{aligned} \quad (32)$$

then the integral

$$\begin{aligned}\int_{-L/2}^{L/2} dx f^* F &= \sum_{n=-\infty}^{\infty} \sum_{n'=-\infty}^{\infty} g_n^* G_{n'} \int_{-L/2}^{L/2} dx e^{2\pi i n' x/L} e^{-2\pi i n x/L} \\ &= L \sum_{n=-\infty}^{\infty} g_n^* G_n\end{aligned}\quad (33)$$

since the integral of the exponentials vanishes whenever $n \neq n'$. Therefore

$$\frac{1}{L} \int_{-L/2}^{L/2} dx f(x)^* F(x) = \sum_{n=-\infty}^{\infty} g_n^* G_n \quad (34)$$

Now, in the $L \rightarrow \infty$ limit I find

$$\begin{aligned}\int_{-\infty}^{\infty} dx f(x)^* F(x) &= \lim_{L \rightarrow \infty} L \sum_{n=-\infty}^{\infty} \frac{h}{2\pi} g^*(k_n) \frac{h}{2\pi} G(k_n) \\ &= \lim_{L \rightarrow \infty} \underbrace{\frac{Lh}{2\pi}}_{=1} \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \delta k g^*(k_n) G(k_n) \\ &= \int_{-\infty}^{\infty} \frac{dk}{2\pi} g(k)^* G(k)\end{aligned}\quad (35)$$

Therefore

$$\int_{-\infty}^{\infty} dx f(x)^* F(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} g(k)^* G(k) \quad (36)$$

For example take $f = \psi$ and $F = d\psi/dx$, then if

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} a(k) e^{ikx} \quad (37)$$

I have

$$F(x) = \frac{df}{dx} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} [ika(k)] e^{ikx} \quad (38)$$

so that $g(k) = a(k)$ and $G(k) = ika(k)$. Then,

$$\int_{-\infty}^{\infty} dx \psi^* \frac{d\psi}{dx} = \int_{-\infty}^{\infty} dx f^* F$$

$$\begin{aligned}
&= \int_{-\infty}^{\infty} \frac{dk}{2\pi} g(k)^* G(k) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} a(k)^* [ika(k)] \\
&= i \int_{-\infty}^{\infty} \frac{dk}{2\pi} k |a(k)|^2
\end{aligned} \tag{39}$$

1.4 Exercises

1. Assume that

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} a(k) e^{ikx} \tag{40}$$

and find the expression for

$$\int_{-\infty}^{\infty} dx f(x) \frac{d^n f(x)}{dx^n} \tag{41}$$

in terms of $a(k)$.

2 Wave packets

There is no reason to limit considerations to 3 dimensions, any function of \mathbf{r}, t can also be expanded in a Fourier series or integral,

$$f(\mathbf{r}, t) = \int \frac{d\omega d^3\mathbf{k}}{(2\pi)^4} g(\mathbf{k}, \omega) e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \tag{42}$$

A note on conventions. The exponent is written as $\omega t - \mathbf{k} \cdot \mathbf{r}$ for the following reason: in quantum mechanics the frequency and wave number are associated with the energy and momentum through $\omega = E/\hbar$, $\mathbf{k} = \mathbf{p}/\hbar$ so that the exponent then reads $(Et - \mathbf{p} \cdot \mathbf{r})/\hbar$ and this expression is relativistically invariant (does not change under a Lorentz transformation).

This is not so for the combination $\omega t + \mathbf{k} \cdot \mathbf{r}$

The wave-function associated with some particle, ψ can be expanded in this fashion

$$\psi(\mathbf{r}, t) = \int \frac{d\omega d^3\mathbf{k}}{(2\pi)^4} \tilde{\phi}(\mathbf{k}, \omega) e^{i(\omega t - \mathbf{k} \cdot \mathbf{r})} \tag{43}$$

At this point this is a purely mathematical statement. In physics, however we will be interested in the *dynamics* of the wave functions.

For example, classical mechanics uses the empirical fact that objects move in space as a result of some external agencies, so their positions can be

described by functions $\mathbf{r}_a(t)$ (a labels the object). among the many brilliant insights of Newton was the realization that these functions are determined from the dynamics, together with the values of all the positions and momenta at one time t_0 ¹. As a result we need to specify $\mathbf{r}_a(t_0), \mathbf{p}_a(t_0)$ together with the expressions for the forces as functions of the positions (and perhaps momenta), and the use Newton's equations to get the time evolution of the system.

Now, in quantum mechanics we do not have position and momenta “coordinates”, instead the full information about the system is contained in its wave function. This has been argued for one particle, but is assumed to be a general statement (as in many of these pronouncements, there is no proof for this postulate, one merely adopts it as a working hypothesis and is satisfied with it only as long as the predictions agree with the observations). So (hopefully), the dynamics of quantum mechanics should tell us what $\psi(\mathbf{r}, t)$ is given the values $\psi(\mathbf{r}, t_0)$ and perhaps $\partial_t \psi(\mathbf{r}, t_0)$ and higher derivatives. Here I will consider only the case where the wave function at time t_0 fully determines the time evolution².

Now, I can take $t_0 = 0$ (equivalent to calling t_0 a convenient time to choose as the origin), the assumption is that $\psi(\mathbf{r}, t)$ is determined from

$$\begin{aligned} \psi(\mathbf{r}, t = 0) &= \int \frac{d\omega d^3\mathbf{k}}{(2\pi)^4} \tilde{\phi}(\mathbf{k}, \omega) e^{-i\mathbf{k}\cdot\mathbf{r}} \\ &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \underbrace{\int \frac{d\omega}{2\pi} \tilde{\phi}(\mathbf{k}, \omega)}_{=\phi(\mathbf{k})} e^{-i\mathbf{k}\cdot\mathbf{r}} \\ &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \end{aligned} \tag{44}$$

so that an equivalent statement is that $\psi(\mathbf{r}, t)$ is uniquely determined by $\phi(\mathbf{k})$ and the equation of motion.

This is a situation similar to that found in electromagnetism: in that case the time evolution is simply obtained by replacing $-\mathbf{k}\cdot\mathbf{r} \rightarrow \omega(\mathbf{k})t - \mathbf{k}\cdot\mathbf{r}$ where $\omega(\mathbf{k})$ is determined from Maxwell's equations and depends on the medium

¹It need *not* be so, for one can imagine a universe where, for example, the initial acceleration of the objects is also needed in order to determine their evolution

²One can hand-wave about this – and I will do so later on, but the ultimate justification for this lies in its experimental success.

the waves travel in. For the vacuum

$$\omega(\mathbf{k}) = c|\mathbf{k}| \quad \text{electromagnetic waves in vacuum} \quad (45)$$

But things can be more complicated: there can be an index of refraction, so that $\omega/|\mathbf{k}| = cn$ and n can depend on \mathbf{k} (as you well know, that is why prisms separate the color in white light: the index of refraction depends on the color). So, in general ω can be a complicated function of \mathbf{k} .

This type of situation also occurs in some quantum systems (though not in all). And I will use it to describe dispersion of waves. Thus I will assume that the quantum dynamics implies that if

$$\psi(\mathbf{r}, t = 0) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \quad (46)$$

then

$$\psi(\mathbf{r}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{i[\omega(\mathbf{k})t - \mathbf{k}\cdot\mathbf{r}]} \quad (47)$$

2.1 Dispersion

I will examine two special cases.

2.1.1 Massless particles

In this case $E = pc$ and, using the deBroglie idea, $\omega = kc$, so that

$$\psi(\mathbf{r}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{ik[ct - \hat{\mathbf{k}}\cdot\mathbf{r}]} \quad (48)$$

Now, write $\phi(\mathbf{k})$ as a function of k and $\hat{\mathbf{k}}$ and imagine first that ϕ is zero except for a narrow set of values centered at $\hat{\mathbf{k}} = \hat{\mathbf{n}}$, in this case

$$\begin{aligned} \psi(\mathbf{r}, t) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(k, \mathbf{n}) e^{ik[ct - \hat{\mathbf{n}}\cdot\mathbf{r}]} \\ &= \int \frac{d\Omega_{\mathbf{n}} k^2 dk}{(2\pi)^3} \phi(k, \mathbf{n}) e^{ik[ct - \hat{\mathbf{n}}\cdot\mathbf{r}]} \\ &= \int \frac{k^2 dk}{(2\pi)^3} e^{ik[ct - \hat{\mathbf{n}}\cdot\mathbf{r}]} \underbrace{\int d\Omega_{\mathbf{n}} \phi(k, \mathbf{n})}_{\chi(k)} \end{aligned}$$

$$= \int \frac{k^2 dk}{(2\pi)^3} \chi(k) e^{ik[ct - \hat{\mathbf{n}} \cdot \mathbf{r}]} \quad (49)$$

In particular ψ is seen to be a function of $ct - \hat{\mathbf{n}} \cdot \mathbf{r}$ only:

$$\psi(\mathbf{r}, t) = f(ct - \hat{\mathbf{n}} \cdot \mathbf{r}) \Rightarrow \psi(\mathbf{r}, 0) = f(-\hat{\mathbf{n}} \cdot \mathbf{r}) \quad (50)$$

so that $\psi(\mathbf{r}, t) = \psi(\mathbf{0}, t - \mathbf{r} \cdot \mathbf{n}/c)$.

this result can be phrased as follows: at time $t = 0$ the wave packet takes the form $\psi(-\mathbf{r} \cdot \mathbf{n}/c)$, at time t the packet looks the same *except* that it is translated by $\mathbf{r} \rightarrow \mathbf{r} - ct\mathbf{n}$: the packet stays the same while traveling at speed c long the direction \mathbf{n} .

2.1.2 General case

Suppose that ω is some known function of k so that

$$\psi(\mathbf{r}, t) = \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{i[\omega(k)t - \mathbf{k} \cdot \mathbf{r}]} \quad (51)$$

Suppose now that ϕ is strongly peaked around $\mathbf{k} = \mathbf{k}_0 = K\mathbf{n}$, so that, writing

$$\mathbf{k} = \mathbf{k}_0 + \mathbf{q} \quad (52)$$

so that for small \mathbf{q} I get

$$\begin{aligned} k &= \sqrt{K^2 + 2K\mathbf{q} \cdot \mathbf{n} + q^2} \\ &= K \sqrt{1 + 2\mathbf{q} \cdot \mathbf{n}/K + q^2/K^2} \\ &= K \left[1 + \frac{\mathbf{q} \cdot \mathbf{n}}{K} + \frac{q^2 - (\mathbf{q} \cdot \mathbf{n})^2}{2K^2} + \dots \right] \\ &= K + \mathbf{q} \cdot \mathbf{n} + \frac{q^2 - (\mathbf{q} \cdot \mathbf{n})^2}{2K} + \dots \end{aligned} \quad (53)$$

Similarly, expanding the exponent

$$\begin{aligned} \omega(k)t - \mathbf{k} \cdot \mathbf{r} &= \left[\omega(K) + \mathbf{q} \cdot \mathbf{n} \frac{d\omega(K)}{dK} + \dots \right] t - (\mathbf{k}_0 + \mathbf{q}) \cdot \mathbf{r} \\ &= \{\omega(K)t - \mathbf{k}_0 \cdot \mathbf{r}\} + \mathbf{q} \cdot [\mathbf{v}_g(K)t - \mathbf{r}] + \dots \end{aligned} \quad (54)$$

where \mathbf{v}_g denotes the group velocity

A note on expansions. The assumption is that ϕ is the fastest changing factor in the integrand, it is not zero near $\mathbf{k} = \mathbf{k}_0$ and vanishes quickly so that the exponent changes by less than 2π as \mathbf{k} moves about the region where ϕ is significantly different from zero. It is not useful to expand ϕ since a power-series approximation does not reproduce a rapid decrease to zero. Note also that the approximation will break down when r and/or t become large enough.

Finally there is the change of variables: $d^3\mathbf{k} = d^3\mathbf{q}$. Putting it all together I get

$$\begin{aligned}\psi(\mathbf{r}, t) &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} \phi(\mathbf{k}) e^{i[\omega(\mathbf{k})t - \mathbf{k} \cdot \mathbf{r}]} \\ &= \int \frac{d^3\mathbf{q}}{(2\pi)^3} \phi(\mathbf{k}_0 + \mathbf{q}) e^{i\{\omega(K)t - \mathbf{k}_0 \cdot \mathbf{r}\} + i\mathbf{q} \cdot [\mathbf{v}_g(K)t - \mathbf{r}] + \dots} \\ &= e^{i\{\omega(K)t - \mathbf{k}_0 \cdot \mathbf{r}\}} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \phi(\mathbf{k}_0 + \mathbf{q}) e^{i\mathbf{q} \cdot [\mathbf{v}_g(K)t - \mathbf{r}] + \dots}\end{aligned}\quad (55)$$

This suggests we define the function

$$f(\mathbf{u}) = \int \frac{d^3\mathbf{q}}{(2\pi)^3} \phi(\mathbf{k}_0 + \mathbf{q}) e^{i\mathbf{q} \cdot \mathbf{u}} \quad (56)$$

in term of which

$$\psi(\mathbf{r}, t) = e^{i\{\omega(K)t - \mathbf{k}_0 \cdot \mathbf{r}\}} f(\mathbf{v}_g(K)t - \mathbf{r}) \quad (57)$$

This implies that except for a phase factor the wave packet travels with velocity $\mathbf{v}_g(K)$ since the argument of f remains constant when $\mathbf{r}/t = \mathbf{v}_g(K)$. So, as long as the approximations used hold, the wave packet behaves as a lump moving along at the group velocity.

2.1.3 Exercises

1. Consider a massless particle with an initial wave-function

$$\psi(\mathbf{r}, t = 0) = A e^{-\mathbf{r}^2/(2R^2)} \quad (58)$$

for some constants A and R . For this system

- (a) Find the corresponding $\phi(\mathbf{k})$

- (b) Find the value of ψ for $t \neq 0$
2. Consider a non-relativistic particle with an initial wave-function

$$\psi(\mathbf{r}, t = 0) = Ae^{-\mathbf{r}^2/(2R^2)} \quad (59)$$

for some constants A and R . For this system

- (a) Find the corresponding $\phi(\mathbf{k})$
- (b) Expand the relativistic expression for the energy $E = \sqrt{m^2c^4 + p^2c^2}$ for $p \ll mc$ to find the non-relativistic expression for the energy as a function of p ; keep terms up to order p^2 and ignore the rest.
- (c) Use the deBroglie relationships to obtain $\omega(k)$ for this system
- (d) Use the general expressions to determine the wave function ψ for $t \neq 0$

Hint: you might find useful the expression

$$\int_{-\infty}^{\infty} dk e^{-uk^2 + vk} = \sqrt{\frac{\pi}{u}} e^{v^2/(4u)} \quad (60)$$

valid whenever the real part of u is non-negative and for all complex v .

2.2 Positin and wave number uncertainties

Imagine that we have a function $f(x)$ that is peaked at $x = 0$ but has a width of order ℓ . Then, if f represent a wave packet we can say that we can specify the position of this packet up to an error of order ℓ . In other words, the *uncertainty* in the position of the wave packet is $\sim \ell$. I will then write

$$\text{Momentum uncertainty} = \Delta x \sim \ell \quad (61)$$

As we saw above this will remain so over time for sufficiently small intervals and distances.

Now consider g the Fourier transform of f ,

$$g(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x) \quad (62)$$

If $|k\ell| \ll 2\pi$ then the exponent is small and varies very little over the region $|x| < \ell$. So in this case we can replace $\exp(-ikx) \simeq 1$:

$$g(k) = \int_{-\infty}^{\infty} dx f(x) \quad |k\ell| \ll 2\pi \quad (63)$$

If, on the other hand $|k\ell| \gg 2\pi$ the exponent will oscillate many times inside the region $|x| < \ell$ where f is appreciably different from zero. Since oscillations alternate in positive and negative values the total result for the integral is very small:

$$g(k) \simeq 0 \quad |k\ell| \gg 2\pi \quad (64)$$

A function that has this behavior (this is *not* a unique possibility but it illustrates well the concepts) is

$$g(k) \sim e^{-[k\ell/(2\pi)]^2} \int_{-\infty}^{\infty} dx f(x) \quad (65)$$

So that the width of g is about $2\pi/\ell$. Again, thinking of g as a wave packet we can say that this width represents the uncertainty of the wave number and I will write

$$\text{Wave-number uncertainty} = \Delta k \sim \frac{2\pi}{\ell} \quad (66)$$

Note that the smaller the uncertainty in the position the larger the uncertainty in the wave number and vice-versa.

This leads to the momentous result

$$\Delta x \Delta k \sim 2\pi \quad \Delta x \Delta p \sim 2\pi\hbar \quad (67)$$

where I used the deBroglie relation between momentum and wave number

This amazing result implies the following:

If one associates a wave to every particle then the momentum and position of all particles cannot be specified with arbitrary precision. The sharper we fix the position the fuzzier is the momentum and vice-versa.

and is known as Heisenberg's uncertainty principle. It is hard to over-emphasize the importance (scientific and philosophical) of this result.